

Exergy and economic analyses of indirect coal-to-liquid technology coupling carbon capture and storage

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ABSTRACT

Coal-to-liquids (CTL) technology has been developed steadily for producing gasoline and diesel fuels as the demand for energy security issue and liquid fuels in China outpaces production capacities. In this light, given the importance of CO₂ emissions in climate change, carbon dioxide capture and storage (CCS) is considered as an integral part of CTL processes. In this study, CTL coupling with CCS technology (CTL-CCS) were simulated using the Aspen Plus software. Based on it, this study conducted exergy and economic analyses to the CTL-CCS system for five different coal types, including anthracite, meager, lean, coking and gas. Results show that the exergy utilization ratios ranged from 40.3% to 43.7%, revealing only a limited effect of the choice of coal type; although anthracite, meager, and gas coal were marginally better. Results also indicate the largest sources of exergy loss to be firstly from gas generation and secondly from the combined process of synthesis and separation. The economic analysis compared the cost, net present value, internal rate of return, and payback period. The cost of liquid fuel produced by CTL-CCS system was in the range from 4117 to 5627 yuan RMB/t, indicating economic feasibility. The system using lean coal revealed the best economic performance, while those using coking coal and gas coal were the second best performers. This research suggests that gas coal can achieve relatively reasonable values for both the exergy utilization ratio and cost in comparison to other coal types processed through a coupled CTL-CCS system.

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1. Introduction

With the global increase in energy demands, petroleum consumption has increased accordingly. As the world's second largest petroleum consumer and the largest petroleum importer, China's energy safety is greatly challenged by its petroleum supply. One of the important responses to the supply crisis lies in establishing a multi-source and diversified petroleum supply system. Coal-to-liquids (CTL) technology producing fuels such as gasoline and diesel from coal is one of the possible candidates in this regard.

At present, coal direct liquefaction project of Shenhua in Erdos is the world's largest single set of large-scale coal direct liquefaction demonstration project. Coal indirect liquefaction demonstration projects in Erdos, Changzhi, and Yulin were put into operation in

2009, 2009 and 2015 respectively (Gu, 2016; Xu, 2015). Another coal indirect liquefaction demonstration project of Shenhua Ningxia Coal Industry Group Co., Ltd has produced oil successfully at the end of December in 2016, which scale is 4 million tons/year (SASAC, 2017). At the end of 2015, the production capacity for coal-to-oil reached 2.54 million tons/year in China. In 2017, the National Energy Administration of China announced the "13th Five-Year" plan for an industrial demonstration of coal deep processing. It is estimated that the production capacity for coal-to-oil will be 13 million tons/year in 2020 (National Energy Administration of China, 2017). According to the plan, four new coal-to-oil demonstration projects will be constructed in China during the period of 13th Five-Year, to undertake 13 demonstration tasks. At the same time, three reserve coal-to-oil projects are considered in Shaanxi, Xinjiang and Ningxia province.

Growing intentions to reduce the serious environmental pollution arising from CO₂ emissions and control the increase in these emissions have been signaled in policies in China recently. One important action taken by the Chinese government is the introduction of national CO₂ intensity reduction targets in China's

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Twelfth Five-Year Plan and Thirteenth Five-Year Plan (17% and 18%, respectively). These are legally binding targets in line with the nation's commitment given in 2009 at the Copenhagen conference on climate change to reduce its CO₂ emission intensity by 40%–45% over the period 2005 to 2020 (News, 2009). Considering that the CTL industry produces a large amount of CO₂, CO₂ capture and storage (CCS) technology can be an important choice for climate change alleviation. Coupling CTL and CCS technology (CTL-CCS) is an obvious choice to simultaneously assure economic benefits from producing a petroleum substitute and reduce CO₂ emissions.

Most recent literature on techno-economic evaluations of CTL-CCS are in general agreement that CTL plants are highly capital intensive but they can be financially viable at sustained high crude oil prices (Bartis et al., 2008; DoE/NETL, 2007; Zhou et al., 2013; Mantripragada and Rubin, 2011). The CO₂ emission of coal liquefaction processes usually can be reduced by co-processing coal and biomass and applying CCS technology, but at the cost of higher capital and operating investments (Srirangan et al., 2012; Tchapda and Pisupati, 2014; Jiang and Bhattacharyya, 2015, 2016, 2017; Kieffer et al., 2016). Most of these studies considered only one kind of coal as the feedstock and only a few discussed which kind of coal might be more suitable or applicable (Mantripragada and Rubin, 2013a, 2013b; Niziolek et al., 2014). The performance and cost of a CTL plant is known to be sensitive to the coal type and gasification technology used (Zhou et al., 2013; Mantripragada and Rubin, 2013c) and more than one kind of coal could be used as raw material in this technology (Hook and Aleklett, 2010).

In China, lignite coal resources account for 5.74% of China's total coal resources; low metamorphic bituminous coal resources account for 51.23% of the total; medium metamorphic bituminous coal (including gas coal, fat coal, coking coal and lean coal) accounts for 28.71% and high metamorphic coal (including meager coal and anthracite coal) accounts for 14.31% (Mao and Xu, 1999). Since these types of coal differ in properties as well as price, research into the implications and economics of CTL-CCS for different coal types has both theoretical value and important practical significance.

In this paper, we will simulate the CTL-CCS system for different types of coal, and provide suggestions on the choice of coal for the CTL-CCS system based on both exergy and economic analysis. The rest of the paper is structured as follows: Section 2 simulate the CTL-CCS system via Aspen Plus software. Section 3 and Section 4 conduct exergy analysis and economic analysis to the CTL-CCS system, respectively. Section 5 discuss the results and conclude the study.

2. Simulation of the CTL-CCS system

Fig. 1 shows the technical route of indirect coal liquefaction coupled with CCS technology. Several processes have not been industrialized yet, so it is necessary to perform simulations, especially for coal gasification and other processes, to assess Fischer–Tropsch (FT) fuels as replacements for traditional liquid fuel.

The technical route considered in this analysis has not been industrialized yet so relevant operating details could not be obtained by measurement. Therefore, it was necessary to obtain data through simulation; Aspen Plus software was selected for this purpose (Tijmensen, 2000; Zhang et al., 2003; Alie, 2004).

In the simulation all systems are divided into subsystems that include the air separation unit (ASU), gasification, the water gas shift (WGS), syngas cleaning, synthesis and distillation, flue-gas cleaning, and power generation. For each unit, different commercial or advanced technologies can be evaluated, compared, and selected. The models for each part are semi-mechanistic and simulated based on selected technologies (Zhou et al., 2013). Shell coal gasification process is selected for our system and simulation (Zhou et al., 2013). This technology is adaptable to many kinds of coal, including lignite, sub bituminous coal, bituminous coal, anthracite and petroleum coke.

Many kinds of coal in China could be chosen as raw material. The Inner Mongolia Province and Xinjiang Province are both major coal producing areas and the main developing areas of the Chinese coal chemical industry. Thus, coal derived from these two provinces was chosen for comparison in this research. These were anthracite coal (760524), meager coal (760527), lean coal (73-1), coking coal (73-6) and gas coal (73-7). The detailed compositions are given in Table 1. Hereafter for simplicity, the specific identification number of each coal type is omitted.

Fig. 2 shows the Simulation flowchart of indirect coal liquefaction coupled with CCS technology (Zhou et al., 2013). Table 2 gives the oil production amount and composition when consuming 1 kg/s of different types of coal. TOPS, KEO and GASOIL represent Gasoline (C5–C10), Kerosene oil (C11–C13), and Diesel oil (C14–C20) products separately.

3. Exergy analysis

Exergy and thermo-economic analyses were first performed in the 1960s (Elsayed and Evans, 1970), and have been reviewed by El-Sayed (2003). The exergy analysis method can be used to evaluate

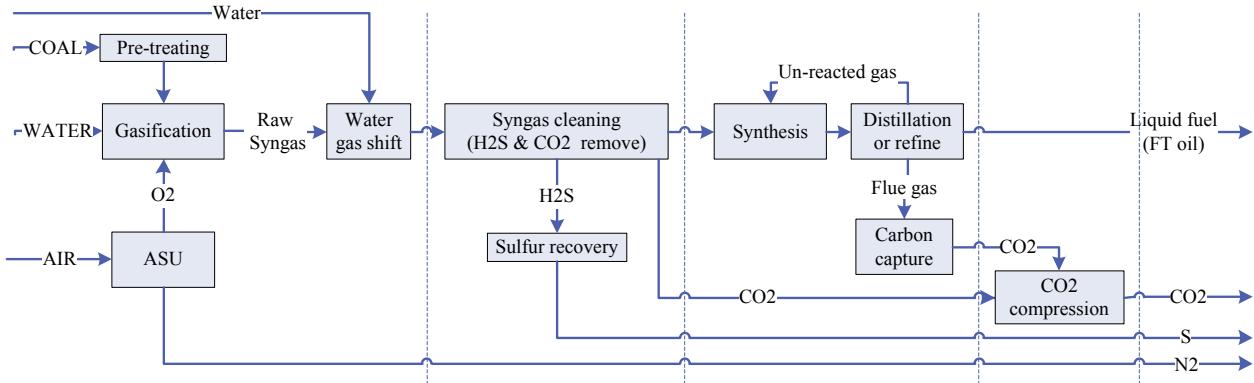
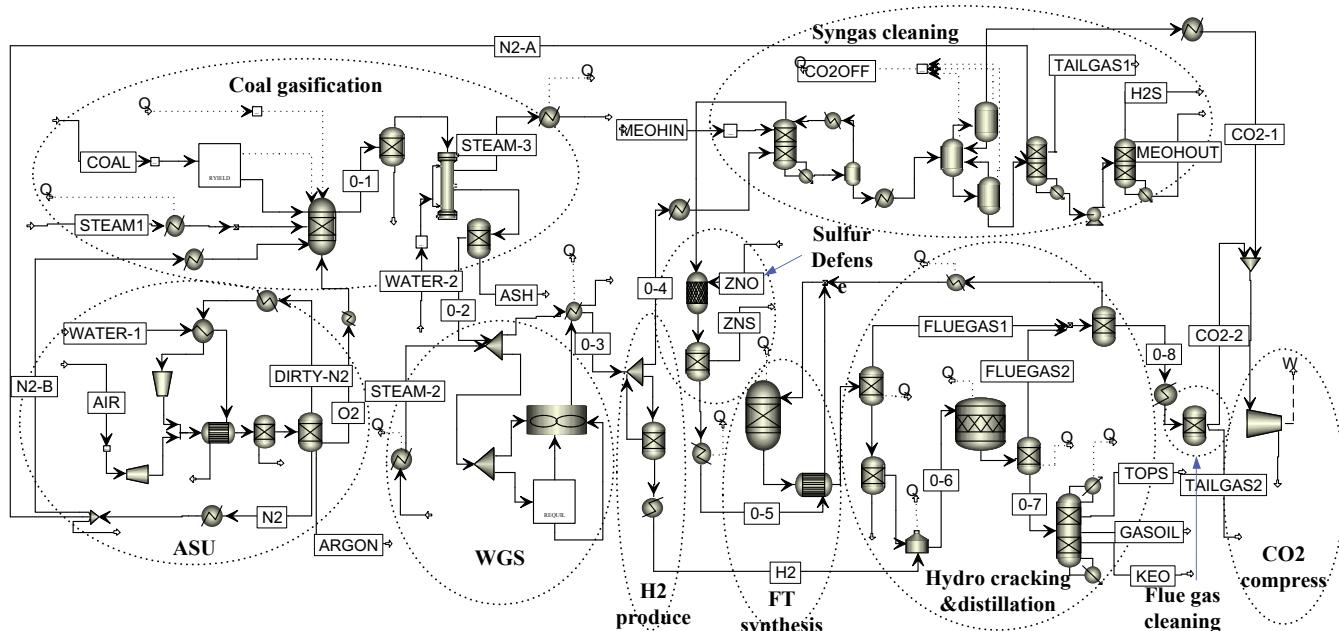


Fig. 1. Indirect liquefaction coupling CCS.

Table 1

Coal composition (dry-basis).

	Mass fraction (%)						Mass fraction (%)			
	Ash	C	H	N	S	O	Water	Fixed carbon	Volatiles	Ash
Anthracite coal (760524)	5.20	90.93	1.13	0.30	0.25	1.27	3.21	88.27	3.32	5.2
Meager coal (760527)	9.81	85.13	3.74	1.23	1.34	2.49	1.57	78.5	10.12	9.81
Lean coal (73-1)	15.63	84.16	4.30	1.46	0.43	3.60	1.47	69.27	13.63	15.63
Coking coal (73-6)	20.57	80.65	4.66	1.23	0.17	2.82	0.93	60.79	17.71	20.57
Gas coal (73-7)	9.45	76.40	5.27	0.99	0.27	11.10	4.12	51.62	34.81	9.45

**Fig. 2.** Simulation flowchart.

the quality changing condition and utilization conditions of energy during an energy utilization process. Exergy is not a standard thermodynamic variable because the exergy of a system is given with respect to local temperature, pressure and composition of the Earth's atmosphere, which vary temporally and spatially. The main objective of exergy analysis is not to calculate an exergy value in a particular state, but rather to deeply research the non-conservative nature of exergy in all kinds of actual processes. Thus, exergy analysis examines the difference between exergy input and exergy output in a system. In a sense, the essence of exergy analysis is the calculation of exergy loss.

3.1. Exergy calculation

The basic implication of exergy is to express the performance ability theoretically. The exergy of a system is the maximum useful work that can be generated during a process that brings the system

into thermal, chemical and mechanical equilibrium with the system's environment. In a broad sense, exergy includes physical exergy (temperature exergy and pressure exergy), chemical exergy (reaction exergy and diffusion exergy) and source and value exergy (electrical exergy and power exergy). In this research, physical exergy (temperature exergy and pressure exergy) and chemical exergy calculations were used.

3.1.1. Physical exergy

Physical exergy includes temperature exergy and pressure exergy.

c_p (kJ/kg·K) is heat capacity. When the system temperature T and the environment temperature T_0 are different, for a process without phase-change, the temperature exergy Ex_t is given by Eq. (1):

Table 2
FT oil production and composition.

	TOPS (kg/sec)	GASOIL (kg/sec)	KEO (kg/sec)	FT oil (kg/sec)
Anthracite coal (760524)	0.044	0.215	0.102	0.361
Meager coal (760527)	0.045	0.219	0.105	0.369
Lean coal (73-1)	0.042	0.204	0.097	0.344
Coking coal (73-6)	0.041	0.199	0.095	0.334
Gas coal (73-7)	0.044	0.211	0.101	0.356

$$Ex_t = \int_{T_0}^T c_p dT - T_0 \int_{T_0}^T \frac{c_p}{T} dT \quad (1)$$

For those processes with phase-change, the latent heat exergy Ex_l should also be taken into consideration using Eq. (2), in which r is the latent heat in the phase-change process:

$$Ex_l = r \left(1 - \frac{T_0}{T} \right) \quad (2)$$

When the system pressure P and the reference pressure P_0 are different, the pressure exergy Ex_p is calculated using Eq. (3). In Eq. (3), R is molar gas constant, and is 8.314 J/(mol·K).

$$Ex_p = RT_0 \ln \frac{P}{P_0} \quad (3)$$

3.1.2. Chemical exergy

Chemical exergy refers to a kind of reversible work when a physical system and its environment reach non-binding equilibrium (in which heat and chemistry reach equilibrium at the same time) from binding equilibrium (i.e., thermodynamic equilibrium). That is, chemical exergy is the exergy of a physical system because of the different composition and environmental conditions.

Generally, the transition of a physical system from binding equilibrium to non-binding equilibrium involves two processes, chemical reaction and physical diffusion. Chemical reaction transforms the original physical system materials into environmental

$$\begin{aligned} Ex_{coal}(CNHSO) = & 34215.87 \times C + 21.97 \times N + 116702.76 \times H + 18260.36 \times S \\ & 13278.59 \times O - 298.15 \times 0.71768 \times M + 0.6276 \times O \times \\ & (32792.8 \times C + 141791.11 \times H - 17723.84 \times O + 16019.49 \times S) \end{aligned} \quad (8)$$

substances; physical diffusion adjusts and diffuses the standard substance concentration into an environmental concentration.

According to the concept of chemical exergy, an environment model is needed. Many researchers have proposed many kinds of models, which are difficult to unify. In this study, the Kameyama-Yoshida model was chosen as it is relatively integrated and has been widely applied (Zhou, 2005). In the model, the temperature T_0 is 25 °C, and the environment pressure P_0 is 1 atm. Moist saturated air is chosen to be the standard substance. The molar gascomposition of N₂, O₂, H₂O, CO₂ and Ar are 0.7560, 0.2034, 0.0312, 0.0003 and 0.0091, respectively. For other elements, the model regards the most stabilized pure substance (liquid state or solid state) as its standard substance. For example, the H element of the model regards liquid water as its standard substance. In modelling a specific environment, the chemical exergy of a compound can be calculated using the exergy balance equation of the formation reaction based on a stabilized simple substance, using existing chemical exergy data of the elements. In this case, only the free enthalpy of formation of the compound must be known. As an example, the compound A_aB_bC_c is assumed to be formed by elements or stabilized simple substance A, B and C. According to the exergy balance equation, the standard chemical exergy of the compound per unit mole in standard state can be determined using Eq. (4).

$$(E_{A_aB_bC_c}) = n_a(E_A)_n + n_b(E_B)_n + n_c(E_C)_n + (\Delta G_f^0)_{A_aB_bC_c} \quad (4)$$

In Eq. (4), E_A , E_B , and E_C are the chemical exergy of A, B and C per unit mole in standard state, respectively; n_a , n_b , and n_c are the moles of A, B and C elements included in the compound, respectively; and $(\Delta G_f^0)_{A_aB_bC_c}$ is the standard free enthalpy of formation of A_aB_bC_c, which can be obtained from a chemical handbook. The standard exergy is modified by the difference between the environment temperature T' and the standard temperature T_0 , and can be calculated using a temperature correction coefficient as illustrated in Eq. (5). The temperature correction coefficient of common compounds ξ can also be obtained from a handbook.

$$E'_{xch}(A_aB_bC_c) = E_{xch}^0(A_aB_bC_c) + \xi(T'_0 - T_0) \quad (5)$$

3.1.3. Other calculations

In addition, syngas, natural gas, and other compounds can be regarded as gas fuel. Their heating value can be used to calculate their exergy approximately because the reaction exergy of fuel is a major proportion of its total chemical exergy. The exergy of other fuels can be approximated similarly. Reaction exergy for gas fuel, liquid fuel and coal can be calculated using Eq. (6), Eq. (7) and Eq. (8), respectively.

$$Ex_G = 0.95 \times HHV \quad (6)$$

$$Ex_L = 0.975 \times HHV \quad (7)$$

In Eqs. (6)–(8), Ex_G , Ex_L and Ex_{coal} are the reaction exergies for gas fuel, liquid fuel and coal, respectively; HHV is the high heating value; C, N, H, S and O are the mass percentages of carbon, nitrogen, hydrogen, sulfur, and oxygen in coal, respectively; and M is the ash content.

The exergy value of water is calculated using Eq. (9) (Zhong et al., 1989):

$$Ex = Ex_0 - 25 \times S_0 \quad (9)$$

In Eq. (9), Ex (kJ/kg) is the exergy value of water at temperature t

Table 3
Values of Ex_0 and S_0 used in this article.

Temperature t/°C	Pressure bar	Ex_0 (kJ/kg)	S_0 (kJ/kg/K)	Ex (kJ/kg)
20	68	13.18	0.4344	2.3
30	68	9.69	0.2949	2.3
300	25	1194.7	6.647	1028.5
20	15	4.42	0.296	-3.0
510	60	1557.6	6.9119	1384.8
200	5	926.8	7.0592	750.3

and pressure p ; and Ex_0 (kJ/kg) and S_0 (kJ/kg/K) are the standard exergy value and entropy value, respectively, of water at temperature t and pressure p . Ex_0 and S_0 can be obtained from a chemical handbook, as shown in Table 3.

3.2. Exergy loss

In this study, the boundary of exergy output and input in the whole system was defined. Input is the consumption of raw materials and electricity in the simulated system and output is oil products produced in the system. In fact, research on the efficiency of exergy utilization is an exergy loss analysis of the system, and shows high efficiency of exergy utilization in the system if the system loses minimal exergy.

In the system, exergy of coal, natural gas and output oil products can be estimated using their heat values because these represent a major proportion of the reaction exergy. The high heating values of gasoline, kerosene and diesel are 46.1, 46.0 and 45.0.

To study the exergy utilization in the simulated system, the system was divided into four parts shown in Fig. 1. These sub-processes are the gas making procedure, syngas cleaning, the synthesis and separation procedure and CO₂ compression.

Using the exergy calculation procedure described in Section 3.1, the exergy utilization for each sub-system and for the total system is shown in Table 4 and Fig. 3.

As shown in Table 4, anthracite coal, meager coal and gas coal could be better choices for the CTL process compared with lean coal and coking coal, considering the exergy utilization ratio. In fact, the types of coal have only a limited effect on the exergy utilization ratio; the total exergy loss of each system is approximately 60%, which means the exergy utilization ratio for each system is approximately 40%. Meanwhile, it should be noted that the flow simulation is simplified. In actual production process, the absolute value might be different effected by the thermal energy and electricity used in each subsystem, conversion ratio, steam cycle efficiency and so on. These changes may have a slight impact on the order of exergy efficiencies. Technical progress of some parts of the system will also influence the results in the future.

The results presented in Table 4 can be compared with those from other systems using coal as a raw material. Gerdes K et al (Gerdes, 2010; Gerdes et al., 2009), and Siefert and Litster (Siefert and Litster) showed that coal-based power plants using integrated gasification combined cycle technology (while sequestering > 90% of the CO₂ generated) can achieve system efficiencies ranging from 32% to 43%. Zhou (2005) calculated that coal-based systems could produce methanol with an efficiency of 40.3% and produce methoxymethane with an efficiency of 43%. Thus, systems producing FT oils are comparable with others in terms of exergy utilization and could be a good choice from this aspect.

As shown in Fig. 3, the largest source of exergy loss is the gas making sub-process and the second largest is the synthesis and separation sub-process. The exergy destruction in the gasifier was significant because there is an inherent mismatch between the

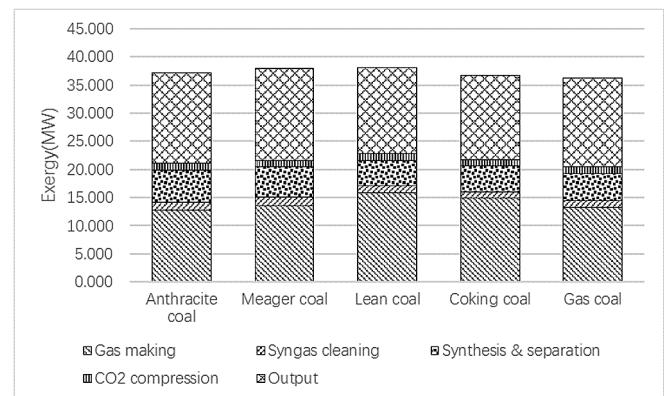


Fig. 3. Exergy destruction and output of systems.

temperature of gasification (1400 °C) and the temperature at which the heat is transferred to the steam (550 °C). Furthermore, the exergy efficiency of the ASU is normally only about 30%–45%. There was also significant exergy destruction in the synthesis and separation sub-process because, even though the temperature of this process is quite high, synthesis and separation is the process where most of the gas is transformed into liquids. From this point of view, improvement of the exergy utilization ratio for the entire CTL process is limited. Some improvements can be achieved, however, and one of the most important is to improve the efficiency by which steam is generated. This can be accomplished by reducing the heat transfer temperature difference.

4. Economic analysis

4.1. Economic estimation model and assumptions

4.1.1. Plant costs

Plant costs are divided into three parts, including process facilities costs (PFC), home office engineering (HOE), and contingency costs. PFC includes investment in main equipment and secondary equipment. The system for indirect coal liquefaction coupling CCS is divided into eleven parts, including coal treatment, coal gasification, air separation, oxygen compressor, WGS, removal of H₂S, removal of CO₂, sulfur recovery, FT synthesis, CO₂ capture after combustion and CO₂ drying and compression. Secondary equipment investment was estimated as a proportion (19.3%) of total main equipment investment.

In order to estimate the equipment investment, the investment data for plant construction could be estimated by a cost index (Peters, 1980) which was chosen as the Chemical Engineering Plant Cost Index. The scale index n relating to the type of equipment is supposed to be between 0.3 and 0.7. It is typically between 0.85 and 0.90 for large-scale production realized by several small-scale equipment in parallel. Based on above assumption, the total

Table 4
Comparison of exergy efficiencies.

Exergy	Input (MW)		Output (MW)		Exergy loss rate (%)	Exergy utilization ratio (%)
	Coal	Electricity	Oil	Compressed CO ₂		
Anthracite coal	32.5	4.63	16.10	0.0251	56.6%	43.4%
Meager coal	33.9	4.10	16.46	0.0250	56.6%	43.4%
Lean coal	34.1	4.01	15.34	0.0250	59.7%	40.3%
Coking coal	33.2	3.51	14.91	0.0250	59.3%	40.7%
Gas coal	33.0	3.35	15.86	0.0250	56.3%	43.7%

Table 5

Calculation of owner costs (Zhou et al., 2013; Zhang et al., 2003).

Total plant investment I_{TPI}	Plant costs I_{PC}	Process facilities costs I_{PFC}	Main equipment investment I_{PE} Secondary equipment investment	Calculated according to Section 3.1 19.3% I_{PE}
		Home office engineering		10% I_{PFC}
		Contingency	Equipment contingency Process contingency	Calculated according to Section 3.1 15% I_{PFC}
		Allowance for funds during construction		Calculated according to cash flow
Owner costs	Raw materials storage Royalty expense Product inventory cost Contractor fees Project study and engineering fees Land-use expenses Working capital Start-up expenses			15 days of coal storage 2% I_{PFC} 0.5% I_{TPI} 1% I_{TPI} 2% I_{TPI} US\$3,000,000 2 months 1 month

investment estimates are calculated by adding all the equipment using Eq. (10):

$$I_{PE} = \sum I_i = \sum \left[\alpha \times I_i^b \times \left(C_i / C_i^b \right)^n \right]. \quad (10)$$

in which I refers to investment, i denotes the i th piece of independent equipment, α refers to the domestic element; C refers to equipment production capacity; superscript b refers to basic data; and n is the scale index. Basic data for equipment and process contingency expenses (Zhou et al., 2013; Kreutz et al., 2005) are obtained from literature. Since the basic data for project costs were in US dollars, the cost data were converted using the dollar–yuan RMB exchange rate data, for which the exchange rate was about 7.0 (Wang, 2009).

HOE includes expenses on project construction management, construction service, and other acceptance and inspection. It can be estimated by a certain percentage of PFC. As recommended in the Electric Power Research Institute (EPRI) model and learned from other study (Zhou et al., 2013), 10% was chosen in this research.

Contingency expenses include two parts, which are project and process contingency expenses. The EPRI guidance recommends that project contingency expenses should be 15%–20% of PFC and 15% is chosen in this study. Process contingency expenses are calculated as the sum of the process contingency expense factors for each piece of equipment.

4.1.2. Owner costs

Owner costs comprise storage costs for raw materials, royalty expenses, product inventory costs, contractor fees, project study and engineering fees, land-use expenses, working capital, and start-up expenses. The basic calculation assumptions for determining these costs are listed in Table 5.

4.1.3. Operational and maintenance costs

Operational and maintenance costs include fixed and variable expenses. Fixed expenses include fixed operational expenses, fixed investment and operational expenses. Fixed operational expenses include enterprise management expenses, taxes, insurance, and basic maintenance expenses. Fixed investment costs include annual interest and fixed capital depreciation. Operational expenses mainly involve labor costs. Variable expenses are mainly related to consumption of raw materials. The calculation method and basic assumptions for operational and maintenance costs are listed in Table 6.

Some basic economic parameters about the system must be assumed for calculating the cash flow. These assumptions (Zhou et al., 2013) are listed in Table 7.

The density of diesel Oil, Gasoline and Kerosene oil are estimated as 0.86 kg/L, 0.739 kg/L and 0.8 kg/L. The price of them are supposed to be 7.1, 6.8 and 4.6 yuan RMB/L when the price of Brent crude oil was about US\$65 per barrel. Then the price of oil is calculated as 7500 yuan RMB/t.

To ensure the consistency of the benchmark, the scale of FT synthesis plants was set at 3,000,000 metric tons of oil products per year. According to the result of process simulation, the raw material consumption for production can be obtained as a proportion of output (see Table 8).

4.2. Evaluation of economic parameters

4.2.1. Cost

The cost of producing oil can be determined using Eq. (11):

$$COST_{oil} = \sum_{i=1}^{COST_i} \left/ \sum_{i=1}^{P_i} \right. \quad (11)$$

Table 6

Calculation method and assumptions (Zhou et al., 2013; Zhang et al., 2003) for operational and maintenance costs.

Fixed expenses	Fixed operational expenses	Enterprise management expenses Taxes and insurance Maintenance expenses	30% of labor expenses 2% I_{PC} + material storage 4% I_{PC} + material storage
	Fixed investment	Interest Fixed capital depreciation	Calculated according to cash flow Calculated according to cash flow
	Operational expenses	Labor expenses	50,000 yuan RMB/person/year
Variable expenses	Other cost Main raw materials expenses Other raw materials expenses		1% of product sales Coal, water, electricity 1% of main raw materials expenses

Table 7
Fixed expenses.

	Unit	Value
Plant construction time	Years	4
Investment rate in various years	Year 1	25%
	Year 2	30%
	Year 3	30%
	Year 4	15%
Equity investment rate	—	20%
Long-term loan interest rate		6.84%
Loan interest rate for short-term capital and current capital	—	6.30%
Discount rate	—	0.125
Project validity	Years	20
Number of employees	Persons	300
Construction commencement rate	Year 1	80%
	1 year later	100%
Sales tax and additional expenses	—	6% of product sales
Income tax	—	25%
Withdrawal of legal surplus public accumulation fund	—	10% of profit
Anthracite coal (760524)	yuan RMB/t	660
Meager coal (760527)	yuan RMB/t	681
Lean coal (73-1)	yuan RMB/t	635
Coking coal (73-6)	yuan RMB/t	617
Gas coal (73-7)	yuan RMB/t	720
Water	yuan RMB/t	2
Electricity	yuan RMB/kWh	0.3
FT oil	yuan RMB/t	7500
Sulfur	yuan RMB/t	800

where $COST_{oil}$, $COST$ and P , respectively, represent the oil product cost, the cash flow cost and oil product output; and i represents the number of operation years of the project.

4.2.2. Net present value

The net present value (NPV) refers to the sum of present values of the benchmark year at the beginning of the calculation period discounted from the net cash flow of each year according to the benchmark discount rate of the industry or other discount rate specified within the economic life (or depreciable life) of the project. The NPV can be determined using Eq. (12):

$$NPV = \sum_{i=1}^n \frac{V_i}{(1+a)^{i-1}} \quad (12)$$

where V represents the net cash flow; i represents the number of operation years of the project; and a represents the discount rate.

For a single project, if $NPV \geq 0$, the project can be considered to be economically viable; if $NPV < 0$, the project shall be rejected. Projects with $NPV \geq 0$ are generally called cost-effective projects, and technologies with $NPV \geq 0$ are generally called cost-effective technologies. In comparisons of multiple projects, the project

with a higher NPV is better (according to the NPV maximum principle).

4.2.3. Internal rate of return

The NPV is calculated according to a specified discount rate and cannot reflect the inherent actual rate of return on investment of a project. Thus, the internal rate of return (IRR) is needed to judge the actual rate of return of a project. In essence, the IRR is the discount rate that makes the total cash outflow equivalent to the total cash inflow accumulated year by year within the whole economic life (or depreciable life) of a project. In other words, IRR is the discount rate at which NPV is zero (Eq. (13)).

$$NPV = \sum_{i=1}^n \frac{V_i}{(1+IRR)^{i-1}} = 0 \quad (13)$$

In practice, IRR must be larger than the benchmark yield or bank loan rate, i.e. $IRR \geq a$. Furthermore, IRR is the largest rate of return of the project. If the loan rate is larger than the IRR, the project will suffer losses. Therefore, IRR reflects the actual return on investment and can be used to determine the minimum economic condition to determine acceptable investment plans.

4.2.4. Payback period

The payback period (PP) refers to the period for recovering investment, i.e. the time needed to recover all investment with the net income, which is equal to annual expenditure from annual income from the commissioning date of the project. The PP can be determined using Eq. (14):

$$PP = I - 1 + \frac{\left| \sum_{i=1}^{I-1} V_i \right|}{V_I} \quad (14)$$

where PP is the payback period; I is the year when the accumulated cash flow begins to have a positive value; V represents the net cash flow; and i represents the year.

4.2.5. Results

The basic economic parameters for the systems are listed in Fig. 4, in which the output of oil is the same amount of 3 million t/year.

As shown in Fig. 4, the cost of liquid fuel produced from the different types of coal were in the range 4117–5627 yuan RMB/t. Recently, when the price of Brent crude oil was about US\$59 per barrel in September 2017, the sale price of Kerosene oil was about 5000–5300 yuan RMB/t ([Energy websit](#)), that of gasoline was about 5.9–6.7 yuan RMB/L, that of diesel oil was 5.5–6.4 yuan RMB/L ([Oil price websit](#)). The average price of Diesel Oil, Gasoline and Kerosene oil could be calculated to be 6.0, 6.3 and 4.1 yuan RMB/L and the sale price of oil produced in these systems is about 6642 yuan RMB/t. Compared with gasoline and diesel oil produced from

Table 8
Raw material consumption and product output of the system.

Type	Consumption			Output	
	Coal	Water	Electricity	Oil products	Sulfur
FT	Anthracite coal	831	1168	38441034	9.98
	Meager coal	813	1143	33351289	50.61
	Lean coal	872	1226	34949183	16.42
	Coking coal	897	1261	31481155	6.76
	Gas coal	846	1190	28342837	10.87

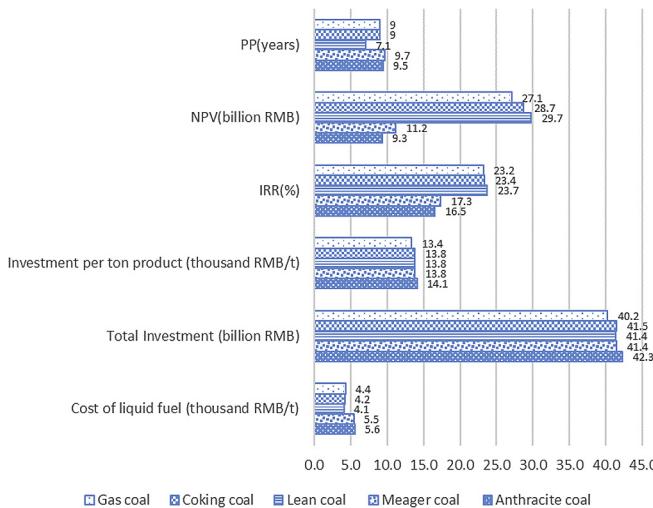


Fig. 4. Basic economic parameters for the FT systems.

crude oil, the results presented in Fig. 4 reveal that coupling of CCS systems to CTL systems can produce fuels that are comparable in price to those produced from crude oil recently.

The largest investment cost per metric ton of product is 5% higher than the smallest cost, and the highest costs of liquid fuel, IRR, NPV and PP are 36.7%, 43.6%, 218%, and 36.6% higher than the respective lowest costs. The coal prices have an obvious influence on the costs and economic benefits of products. Among the types of coal evaluated, lean coal seems to be the best choice on an economic basis, followed in order by coking coal and gas coal. Anthracite coal is the least suitable choice. It could be further estimated that when the price of Brent crude oil was lower than US\$38 per barrel, there is no economic benefit even using lean coal as raw material. Meanwhile, it should be noted that the data of assumption could be different. These absolute value of results could also be influenced especially by the price of CO₂ emissions, coal and oil. However, relative order will not change a lot.

5. Conclusions

In this study, exergy and economic analyses were conducted to examine the use of five different types of coal in the CTL process coupled with CCS. Aspen Plus software was used to simulate the coupled CTL-CCS technology. Using the flow simulation results for the five types of coal, exergy data and financial indicators were determined.

The exergy utilization analysis showed system efficiency in the range 40.3%–43.7%, which was similar to the value reported by others for systems using coal as raw material to produce electricity, methanol or methoxymethane. In fact, the type of coal used in the CTL-CCS process has only a limited effect on exergy utilization ratio. Efficiencies of systems using anthracite coal, meager coal and gas coal were about 43%, while efficiencies from the use of lean coal and coking coal approximated 40%. As indicated by the exergy destruction and output of systems, the largest source of exergy loss is the gas making sub-process and the second largest is the combined synthesis and separation sub-process. One of the most important ways to reduce exergy loss is to improve the efficiency by which steam is generated, and this can be accomplished by reducing the heat transfer temperature difference. More, environmental burden is also very important. One of the aspects is about the impact of waste and emissions. The exergy loss would occur in dealing with them until they have no influence on the

environment. After more processes will be industrialized in the future, more discussion about environmental burden will be useful to improve the understanding of the system.

The economic analysis of the various types of coal inputs showed the cost of liquid fuel to be in the range 4117–5627 yuan RMB/t. Compared with the cost of producing liquid fuel products from crude oil, the economic analysis revealed that coupling of CCS systems to indirect coal liquefaction systems is economically feasible when the international crude oil price is higher than US\$ 50 per barrel. From an international perspective, the CO₂ emissions tax is considered to be €15–20 per ton (Bruvoll and Bodil, 2004; Wier et al., 2005) (150–200 yuan RMB/t). As pressure to reduce CO₂ emissions increases, coupling of CCS to FT synthesis technology can be expected to become more economically competitive. Among different types of coal examined, the system using lean coal resulted in the lowest cost of liquid fuel, investment and payback period, and the highest IRR and NPV. Therefore, FT synthesis using lean coal can provide the best results from a cost-benefit perspective, while production using coking coal or gas coal could be a good second choice.

Exergy utilization ratio of gas coal is highest, while system using it has lowest investment and medium cost of liquid fuel. When considering these two aspect equally, this research suggests that coupling of CCS to FT synthesis technology using gas coal can achieve both relatively the most reasonable values for the exergy utilization ratio and economic benefit in comparison to the use of other coal types. The calculations suggest that there may be scenarios in which coupling of CCS to FT synthesis technology is economically viable, meriting further research and development of these technologies.

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